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A micromechanics-based approach for the derivation of constitutive elastic coefficients of strain-gradient media

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ABSTRACT

A micromechanics-based approach for the derivation of the effective properties of periodic linear elastic composites which exhibit strain gradient effects at the macroscopic level is presented. At the local scale, all phases of the composite obey the classic equations of three-dimensional elasticity, but, since the assumption of strict separation of scales is not verified, the macroscopic behavior is described by the equations of strain gradient elasticity. The methodology uses the series expansions at the local scale, for which higher-order terms, (which are generally neglected in standard homogenization framework) are kept, in order to take into account the microstructural effects. An energy based micro–macro transition is then proposed for upscaling and constitutes, in fact, a generalization of the Hill–Mandel lemma to the case of higher-order homogenization problems. The constitutive relations and the definitions for higher-order elasticity tensors are retrieved by means of the "state law" associated to the derived macroscopic potential. As an illustration purpose, we derive the closed-form expressions for the components of the gradient elasticity tensors in the particular case of a stratified periodic composite. For handling the problems with an arbitrary microstructure, a FFT-based computational iterative scheme is proposed in the last part of the paper. Its efficiency is shown in the particular case of composites reinforced by long fibers.

1. Introduction

Conventional homogenization processes applied to periodic composite materials generally use the assumption of scale separation, i.e. the size of microstructural elements remains negligible compared with the size of the studied mechanical components or with the characteristic length of the applied load. Under this hypothesis, the macroscopic quantities are nearly constant at local scale (the scale of the heterogeneities) and the effective properties, obtained from the homogenization procedure, do not introduce the size of the microstructural elements, typically, the size of inclusions or the size of the periodic unit cell. This framework is valid in many situations, specially when the heterogeneities are micrometer sized and when the gradient of the macroscopic strain remains small enough. When such assumptions are not satisfied, the size of the microstructural elements affects the macroscopic behavior of composites. Moreover, these effects can become predominant for some special practical problems in mechanics and of high importance for structural design such as in the case of fracture (see Exadaktylos, 1998; Altan and Aifantis, 1992; Georgiadis and Grentzelou, 2006) or the localization phenomenon (see Triantafyllidis and Aifantis, 1986; Chambon et al., 2001; Engelen et al., 2006) for which very large values of strain gradient may occur.

Generalized continuum-mechanics theories introduce a characteristic length of the microstructure, (Toupin, 1962, 1964; Mindlin, 1964; Mindlin and Eshel, 1968), (see Fleck and Hutchinson, 1993; Fleck et al., 1994; Mühlhaus and Aifantis, 1991 for a plastic version of the strain gradient models). These approaches extend the usual linear elasticity by including the gradient of strain and higher-order derivatives of the strain in the expression of the elastic energy density. These models are often considered as describing more adequately the effect of the microstructure at the macroscale. However they are phenomenological in the sense that the constitutive elastic coefficients are not derived from a micromechanics-based framework. Moreover, such models generally introduce a large number of coefficients whose identification constitutes an important limitation for their use in the modeling of structures.

The derivation of the constitutive equations of non local models in a homogenization framework has been the subject of extensive research during the last three decades. Among the first, (Diener et al., 1981, 1982, 1984) and later (Drugan and Willis, 1996) derived a non local constitutive model from the variational Hashin–Shtrikman variational principle. Other works, (Bouyge et al., 2001, 2002; Kouznetsova et al., 2002, 2004; Yuan

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et al., 2008) have used higher-order boundary type conditions for the unit cell in order to derive the constitutive equations of generalized continuum models. These approaches use a generalization of the Hill–Mandel's macrohomogeneity condition for deriving the higher-order constitutive relations and can deal with non-linear materials while the present paper offers only developments in the linear elastic case. However, as mentioned by Yuan et al. (2008), these definitions produce overevaluated values of the macroscopic internal energy of gradient elastic media and give rise to some unphysical results. Indeed, the macroscopic behavior obtained from this procedure still leads to a macroscopic gradient elastic model even if the unit cell is defined by a homogeneous material.

Still in the context of periodic microstructures, Gambin and Kroener (1989), Boutin (1996), Triantafyllidis and Bardenhagen (1996) and later Smyshlyaev and Cherednichenko (2000) have studied the influence of the higher-order terms of the series expansion on the macroscopic behavior of linear elastic composites. This approach of series expansion, which has been initiated by Bensoussan et al. (1978) and Sanchez-Palencia (1980), has shown to be a rigorous and efficient method for introducing the effect of the macroscopic gradient of strain on the local response of linear composites. The asymptotic expansion method introduces the scale factor ϵ defined as the ratio between the characteristic length of the microstructure and the one of the applied macroscopic loading. When this scale factor ϵ is very small compared with 1, there is a strict separation of the micro and macroscopic scales. In practice, the limit $\epsilon \to 0$ is taken in the expression of strains and stresses, and the standard homogenization framework can be used. When the parameter ϵ is close to 1, no homogenization is valid anymore. When ϵ is lower than 1 but not negligible before 1, the solution can be approximated by keeping higher-order terms in the series expansion. All these terms are then obtained by solving a hierarchy of higher-order elasticity problems with prescribed body forces and eigenstrains whose expressions depend on the solution at the lower-order. In Boutin (1996), the author does not interpret the macroscopic response of the composite as of strain gradient type but only considers the higher-order terms of the series in order to evaluate the deviation of the macroscopic stress–strain relation from the classic one, due to the microstructural effects. Later Smyshlyaev and Cherednichenko (2000) also studied the higher-order terms of the asymptotic expansion in the framework of variational principles and showed that the resulting "homogenized model", with the appropriate definitions for the macroscopic quantities, leads to constitutive equations which are in agreement with the gradient elasticity theories. In the present paper we propose a simple method for computing the effective properties of elastic composites which exhibit a gradient effect at the macroscopic scale which depends on a characteristic length of the microstructure. The method follows the "asymptotic based" approaches of Boutin (1996), Smyshlyaev and Cherednichenko (2000). The transition between the micro and macro scales is effected by defining the macroscopic elastic energy density as the average of the local energy density: this can be interpreted as a generalization of the Hill–Mandel Lemma for higher order homogenization problems, similarly to the works of Bouyge et al. (2001) and Yuan et al. (2008). The macroscopic law of the composite is then obtained by means of the "state law" associated to the macroscopic potential. As an illustration, we derive the closed-form solution for the higher-order elastic coefficients in the case of a periodic stratified composite. For handling the problem of an arbitrary geometry of the unit cell, we extend the FFT-based method initially introduced for elasticity by Moulinec and Suquet (1994). The ability of this numerical approach is illustrated in the case of a composite made up of periodically aligned fibers along a regular network.

2. Higher-order homogenization problems and their solutions

In this section, we recall shortly without new developments the asymptotic expansion method applied to periodic composites and its elastic solution as derived in the work of Boutin (1996), because this work constitutes the basis of the developments proposed in the present paper. Let us consider a periodic microstructure defined by a parallelepipedic unit cell Y and three vectors denoted by $\boldsymbol{d}_1$, $\boldsymbol{d}_2$, $\boldsymbol{d}_3$ which characterize the translational invariance. Each constituent obeys the equations of three-dimensional elasticity:

$$\begin{cases} \nabla_z \cdot \boldsymbol{\sigma} + \boldsymbol{f}(z) = 0 \\ \boldsymbol{\sigma} = \boldsymbol{c}(z) : \boldsymbol{\varepsilon} \\ \boldsymbol{\varepsilon} = \frac{1}{2}(\nabla_z \otimes \boldsymbol{u} + \boldsymbol{u} \otimes \nabla_z) \end{cases} \tag{1}$$

where $z = (z_1, z_2, z_3)$ denotes the vector position. By $\boldsymbol{c}(z)$, we denote the fourth-order elasticity tensor of the periodic composite which is piecewise constant and invariant by any translation according to the vectors $\boldsymbol{d}_1$, $\boldsymbol{d}_2$, $\boldsymbol{d}_3$. The inclusions and the matrix are assumed to be perfectly bonded through their interfaces. Then, the displacement field, $\boldsymbol{u}$, and the traction vector, $\boldsymbol{t} = \boldsymbol{\sigma} \cdot \boldsymbol{n}$, remain continuous across the interface between the matrix and the heterogeneities. The problem is defined by its two characteristic length scales, h and L. The first, h, is characteristic of the microstructural elements (the size of the unit cell, of the inclusions, the distance between two neighboring inclusions...). L denotes a characteristic length of the studied macrostructure or the characteristic size related to the applied load. The ratio between these two lengths defines the scale factor, $\epsilon = h/L$ which is assumed to be smaller than 1 but not negligible. The existence of a small parameter in (1) allows to search the solution along asymptotic series. The technique basically consists in four steps:

- The presence of two length scales suggests to introduce the non dimensional space variables $x = z/L$ and $y = z/h$, where x is the "slow" oscillating variable while y is the "fast" oscillating variable.
- The displacement field is expanded as a power series in ϵ:

$$\boldsymbol{u}(x,y) = L\sum_{i=0}^{+\infty} \epsilon^i \boldsymbol{u}^i(x,y) \tag{2}$$

where the displacements fields $\boldsymbol{u}^i(x,y)$ are Y-periodic and non dimensional due to the presence of the lengthscale L before the sum in the previous equation.

- The gradient operator is decomposed into two parts: $\nabla_z = \frac{1}{L}(\nabla_x + \frac{1}{\epsilon}\nabla_y)$, where the indices x and y indicate that the derivatives are taken respectively with respect to x and y.
- By equating terms with the same power of ϵ, we get a hierarchy of equations for the quantities $\boldsymbol{u}^0(x,y)$, $\boldsymbol{u}^1(x,y)$, $\boldsymbol{u}^2(x,y)$, etc.

The total displacement field takes the form:

$$\boldsymbol{u}(x,y) = \boldsymbol{U}(x) + \epsilon \boldsymbol{X}^1(y) : \boldsymbol{E}(x) + \epsilon^2 \boldsymbol{X}^2(y) : \cdot \boldsymbol{G}(x) + \epsilon^3 \boldsymbol{X}^3(y) :: \boldsymbol{D}(x) \ldots \tag{3}$$

In which quantities $\boldsymbol{U}(x)$, $\boldsymbol{E}(x)$, $\boldsymbol{G}(x)$ and $\boldsymbol{D}(x)$ are functions of the variable x while tensors $\boldsymbol{X}^1(y)$, $\boldsymbol{X}^2(y)$, ... are only functions of the variable y. Tensors $\boldsymbol{X}^1(y)$, $\boldsymbol{X}^2(y)$, ... are obtained by solving a hierarchy of linear elasticity problems which are given in Appendix A. The physical meaning of quantities $\boldsymbol{U}(x)$, $\boldsymbol{E}(x)$, $\boldsymbol{G}(x)$ and $\boldsymbol{D}(x)$ will be specified in the next section.

The associated strain field is:

$$\boldsymbol{\varepsilon}(x,y) = \boldsymbol{a}^0(y) : \boldsymbol{E}(x) + \epsilon \boldsymbol{a}^1(y) : \cdot \boldsymbol{G}(x) + \epsilon^2 \boldsymbol{a}^2(y) :: \boldsymbol{D}(x) \ldots \tag{4}$$

where the components of tensors $\boldsymbol{a}^0(y)$, $\boldsymbol{a}^1(y)$, etc., are related to the ones of tensors $\boldsymbol{X}^1(y)$, $\boldsymbol{X}^2(y)$, etc., by:

$$
\begin{aligned}
a^0_{ijpq}(y) &= \frac{1}{2}\left(\delta_{ip}\delta_{jq} + \delta_{iq}\delta_{jp}\right) + \frac{1}{2}\left\{\frac{\partial X^1_{ipq}}{\partial y_j}(y) + \frac{\partial X^1_{jpq}}{\partial y_i}(y)\right\}\\
a^1_{ijpqr}(y) &= \frac{1}{2}\left\{X^1_{ipq}(y)\delta_{jr} + X^1_{jpq}(y)\delta_{ir}\right\} + \frac{1}{2}\left\{\frac{\partial X^2_{ipqr}}{\partial y_j}(y) + \frac{\partial X^2_{jpqr}}{\partial y_i}(y)\right\}\\
&\text{etc.}
\end{aligned} \tag{5}
$$

The local stress field reads:

$$\boldsymbol{\sigma}(x,y) = \boldsymbol{c}^0(y) : \boldsymbol{E}(x) + \epsilon \boldsymbol{c}^1(y) : \cdot \boldsymbol{G}(x) + \epsilon^2 \boldsymbol{c}^2(y) : \cdot \boldsymbol{D}(x) \dots \tag{6}$$

with $\boldsymbol{c}^\alpha(y) = \boldsymbol{c}(y){:}\boldsymbol{a}^\alpha(y)$. The local fields then require the identification of the components of tensors $\boldsymbol{X}^\alpha(y)$ for $\alpha \geqslant 1$.

3. The micro–macro transition

In this section, we propose a homogenization process based on the elastic energy density which proves to be adapted for taking properly into account higher order terms of the asymptotic series and the microstructural effects at the macroscopic level. As in the standard thermodynamic framework, the macroscopic law is obtained by means of the state law associated to the derived expression of the homogenized elastic potential. It is shown that the resulting macroscopic model complies with the first gradient theory of Toupin (1962, 1964) and Mindlin (1964, 1968), when the series is truncated at the second order, and allows to recover the more general gradient elastic theory established by Green and Rivlin (1964), when all the terms of the series are kept.

3.1. Definitions for the stress and hyperstress

Since all tensors $\boldsymbol{X}^\alpha(y)$ in (3) have a null volume average over a period, it follows that:

$$\langle \boldsymbol{u}(x,y)\rangle_V = \boldsymbol{U}(x) \tag{7}$$

$\boldsymbol{U}(x)$ represents the macroscopic displacement field which can be interpreted as the translation of the geometric center of the unit cell. Taking into account the following equalities:

$$\langle \boldsymbol{a}^0(y)\rangle_V = \boldsymbol{I}; \quad \langle \boldsymbol{a}^\alpha(y)\rangle_V = 0 \quad \alpha = 1,2,\dots \tag{8}$$

where $\boldsymbol{I}$ denotes the Fourth order identity tensor, it follows that the average of the local strain is given by:

$$\langle \boldsymbol{\varepsilon}(x,y)\rangle_V = \boldsymbol{E}(x) = \frac{1}{2}(\nabla_x \otimes \boldsymbol{U}(x) + \boldsymbol{U}(x) \otimes \nabla_x) \tag{9}$$

$\boldsymbol{E}(x)$ is then interpreted as the macroscopic strain and $\boldsymbol{G}(x)$ and $\boldsymbol{D}(x)$ are respectively the non-dimensional gradient and double gradient of macroscopic strain, the derivative being taken according to the non dimensional macroscopic vector position, x. It follows that, in all the expressions, $\epsilon\boldsymbol{G}(x)$ and $\epsilon^2\boldsymbol{D}(x)$ must be replaced by: $h\nabla\boldsymbol{E}(x)$ and $h^2\nabla^2\boldsymbol{E}(x)$. Taking into account the expression of the total strain and stress fields (see Eqs. (4) and (6)), the average of the local density energy over the volume of the unit cell can be written in the form:

$$
\begin{aligned}
W(x) &= \frac{1}{2}\langle \boldsymbol{\sigma}(x,y) : \boldsymbol{\varepsilon}(x,y)\rangle_V = \frac{1}{2}\sum_{\alpha=0}^{\alpha=+\infty}\sum_{\beta=0}^{\beta=+\infty} h^{\alpha+\beta}\nabla^\alpha \boldsymbol{E}(x) : \boldsymbol{C}^{\alpha,\beta} : \nabla^\beta \boldsymbol{E}(x)\\
&= \frac{1}{2}\Big\{\boldsymbol{E}(x) : \boldsymbol{C}^{0,0} : \boldsymbol{E}(x) + 2h\boldsymbol{E}(x) : \boldsymbol{C}^{0,1} : \nabla\boldsymbol{E}(x) + h^2\nabla\boldsymbol{E}(x) : \boldsymbol{C}^{1,1} : \nabla\boldsymbol{E}(x)\\
&\quad + 2h^2\boldsymbol{E}(x) : \boldsymbol{C}^{0,2} : \nabla^2\boldsymbol{E}(x) + 2h^3\nabla\boldsymbol{E}(x) : \boldsymbol{C}^{1,2} : \nabla^2\boldsymbol{E}(x)\\
&\quad + 2h^3\nabla\boldsymbol{E}(x) : \boldsymbol{C}^{0,3} : \nabla^3\boldsymbol{E}(x) + \cdots\Big\}
\end{aligned} \tag{10}
$$

with:

$$C^{\alpha,\beta}_{i\dots jp\dots q} = \langle c^\alpha_{kli\dots j}(y) a^\beta_{klp\dots q}(y)\rangle_V = \langle c_{klmn}(y) a^\alpha_{mni\dots j}(y) a^\beta_{klp\dots q}(y)\rangle_V \tag{11}$$

where the $\boldsymbol{C}^{\alpha,\beta}$ are tensors of order $\alpha + \beta + 4$. Note that tensor $\boldsymbol{C}^{\beta,\alpha}$ can be seen as the "transpose" of $\boldsymbol{C}^{\alpha,\beta}$ obtained by permuting the first $\alpha + 2$ indices with the last $\beta + 2$ indices. The quantity $W(x)$ is called thereafter macroscopic elastic energy. It can be observed that $W(x)$ is a quadratic function according to the macroscopic quantities $\boldsymbol{E}(x),\ \nabla\boldsymbol{E}(x),\ \nabla^2\boldsymbol{E}(x)$, etc. As usually in the thermodynamic framework, it is possible to define the dual variables associated to $\boldsymbol{E}(x),\ \nabla\boldsymbol{E}(x),\ \nabla^2\boldsymbol{E}(x)$, by means of the state law:

$$
\begin{aligned}
\boldsymbol{\Sigma}(x) &= \frac{\partial W}{\partial \boldsymbol{E}} = \langle \boldsymbol{\sigma}(x,y){:}\boldsymbol{a}^0(y)\rangle_V\\
&= \boldsymbol{C}^{0,0}{:}\boldsymbol{E}(x) + h\boldsymbol{C}^{0,1}{:\cdot}\nabla\boldsymbol{E}(x) + h^2\boldsymbol{C}^{0,2}{::}\nabla^2\boldsymbol{E}(x) + \cdots\\
\boldsymbol{T}(x) &= \frac{\partial W}{\partial \nabla\boldsymbol{E}} = h\langle \boldsymbol{\sigma}(x,y){:}\boldsymbol{a}^1(y)\rangle_V\\
&= h\boldsymbol{C}^{1,0}{:}\boldsymbol{E}(x) + h^2\boldsymbol{C}^{1,1}{:\cdot}\nabla\boldsymbol{E}(x) + h^3\boldsymbol{C}^{1,2}{::}\nabla^2\boldsymbol{E}(x) + \cdots\\
\boldsymbol{M}(x) &= \frac{\partial W}{\partial \nabla^2\boldsymbol{E}} = h^2\langle \boldsymbol{\sigma}(x,y){:}\boldsymbol{a}^2(y)\rangle_V\\
&= h^2\boldsymbol{C}^{2,0}{:}\boldsymbol{E}(x) + h^3\boldsymbol{C}^{2,1}{:\cdot}\nabla\boldsymbol{E}(x) + h^4\boldsymbol{C}^{2,2}{::}\nabla^2\boldsymbol{E}(x) + \cdots \text{etc.}
\end{aligned} \tag{12}
$$

$\boldsymbol{\Sigma}(x)$ is the macroscopic stress and $\boldsymbol{T}(x)$, $\boldsymbol{M}(x)$, etc., are called hyperstresses. Tensors $\boldsymbol{C}^{\alpha,\beta}$ are the elastic tensors of the generalized continuum whose determination requires the computation of functions $\boldsymbol{X}^\alpha(y)$ for $\alpha = 1, 2, 3, \dots$ Let us recall that these tensors are determined by solving successively a hierarchy of linear elastic problems also called "higher order homogenization problem" in the literature and which can be found in Appendix A. The problems can be solved by standard numerical tools as the Finite Element Method (FEM) or, as proposed in Section 5, by a Fast Fourier transform based numerical approach, adapted to the context of the computational homogenization of periodic structures.

It must be emphasized that the macroscopic stress is not defined by the classic volume average, $\boldsymbol{\Sigma}(x) \neq \langle \boldsymbol{\sigma}(x,y)\rangle_V$. This constitutes an important difference with Boutin (1996), together with the fact that the hyperstresses have not been introduced in Boutin's work. With the above definitions, it follows that:

$$\langle \boldsymbol{\sigma}(x,y) : \boldsymbol{\varepsilon}(x,y)\rangle_V = \boldsymbol{\Sigma}(x) : \boldsymbol{E}(x) + \boldsymbol{T}(x) : \cdot\nabla\boldsymbol{E}(x) + \boldsymbol{M}(x) :: \nabla^2\boldsymbol{E}(x) + \cdots \tag{13}$$

which constitutes a generalization of the Hill–Mandel lemma to higher-order homogenization framework. For completeness, we have to demonstrate that the stress and hyperstresses (12) comply with the balance equation for such models of generalized continua. This is the subject of the following sub-section. Before proceeding to this, let us provide the following remarks:

(a) When the limit $h \to 0$ of the macroscopic potential (10) is taken, all terms associated to the gradient of strain and to higher order derivatives vanish and the energy density reduces to $W(x) = \frac{1}{2}\boldsymbol{E}(x) : \boldsymbol{C}^{0,0} : \boldsymbol{E}(x)$. The macroscopic elastic law reduces to $\boldsymbol{\Sigma}(x) = \boldsymbol{C}^{0,0} : \boldsymbol{E}(x)$. Obviously, the resulting macroscopic model is of Cauchy type and the standard equations for homogenization are recovered.

(b) When all the series are truncated at the order 1 in the expression of the microscopic strain field (4), the macroscopic elastic energy density $W(x)$ computed from (10) takes the form:

$$
\begin{aligned}
W(x) &= \frac{1}{2}\boldsymbol{E}(x) : \boldsymbol{C}^{0,0} : \boldsymbol{E}(x) + h\boldsymbol{E}(x) : \boldsymbol{C}^{0,1} : \nabla\boldsymbol{E}(x)\\
&\quad + \frac{h^2}{2}\nabla\boldsymbol{E}(x) : \boldsymbol{C}^{1,1} : \nabla\boldsymbol{E}(x)
\end{aligned} \tag{14}
$$

which can be interpreted as the energy density introduced in the first strain gradient theories of Toupin (1962, 1964), Mindlin (1964), Mindlin and Eshel (1968). Note also that a truncature at the order 2 in the expression of the microscopic strain field (4), leads to a macroscopic energy density which is quadratic with respect to the macroscopic strain, gradient of strain and double gradient of macroscopic strain. Such a potential can be interpreted as the energy density of the second strain gradient theory of Mindlin (1965).

(c) When all the terms of the series are kept in the expression of the microscopic strain field (4), the macroscopic energy density is the one introduced in a more general theory established by Green and Rivlin (1964) which includes the derivatives of the strain at any order.

3.2. The macroscopic balance equation

In this section we prove that the definitions of the stress and of the hyperstresses (12) are compatible with the balance equation of elastic strain gradient continua. To this end, let us start from the local balance equation with the decomposition $\nabla_z = \frac{1}{L}(\nabla_x + \frac{1}{\epsilon}\nabla_y)$:

$$\nabla_x \cdot \boldsymbol{\sigma} + \frac{1}{\epsilon}\nabla_y \cdot \boldsymbol{\sigma} + \boldsymbol{f}(x,y) = 0 \tag{15}$$

The traction $\boldsymbol{\sigma}\cdot\boldsymbol{n}$ at the boundary of the unit cell is Y-antiperiodic. The volume average of the quantity $\nabla_y \cdot \boldsymbol{\sigma}$ is then equal to zero and:

$$\nabla_x \cdot \langle\boldsymbol{\sigma}\rangle_V + \boldsymbol{F}(x) = 0 \tag{16}$$

where we have denoted $\boldsymbol{F}(x) = \langle \boldsymbol{f}(x,y) \rangle_V$ and $\langle\boldsymbol{\sigma}\rangle_V$ is only a function of the macroscopic variable x. In the classic homogenization framework, the series in (6) is truncated at the zero order and $\langle\boldsymbol{\sigma}\rangle_V$ represents the macroscopic stress tensor, $\boldsymbol{\Sigma}(x)$. In that case, Eq. (16) reduces to $\nabla_x \cdot \boldsymbol{\Sigma}(x) + \boldsymbol{F}(x) = 0$ which means that the macroscopic law of the composite is of Cauchy type. When higher order terms are kept in the series (6), the quantity $\langle\boldsymbol{\sigma}\rangle_V$ cannot be interpreted as the macroscopic stress since the definitions (12) are now used. However, a representation of the average $\langle\boldsymbol{\sigma}\rangle_V$ in terms of the macroscopic quantities $\boldsymbol{\Sigma}(x)$, $\boldsymbol{T}(x)$, $\boldsymbol{M}(x)\ldots$ is possible. Starting from the definitions of the macroscopic stress (12) and of the localization tensor $\boldsymbol{a}^0(y)$ given by (5), one has, for $\alpha \geqslant 0$:

$$\frac{1}{V}\int_V \sigma_{pq} a^{\alpha}_{pqi\ldots jk}(y)dV = \frac{1}{V}\int_V \sigma_{pk} X^{\alpha}_{pi\ldots j}(y)dV + \frac{1}{V}\int_V \sigma_{pq}\frac{\partial X^{\alpha+1}_{pi\ldots jk}}{\partial y_q}(y)dV \tag{17}$$

where X^0_{ij} is conventionally taken as $X^0_{ij}(y) = \delta_{ij}$. Using the divergence theorem and accounting for $\partial/\partial y_i = -\epsilon\partial/\partial x_i$, one has:

$$\frac{1}{V}\int_V \sigma_{pq}\frac{\partial X^{\alpha+1}_{pi\ldots jk}}{\partial y_q}(y)dV = \frac{1}{V}\int_{\partial V} \sigma_{pq} n_q X^{\alpha+1}_{pi\ldots jk}(y)dV + \epsilon\frac{\partial}{\partial x_q}\left\{\frac{1}{V}\int_V \sigma_{pq} X^{\alpha+1}_{pi\ldots jk}(y)dV\right\} \tag{18}$$

The first term at the right of the above equality is null, due to the periodicity of $X^{\alpha+1}_{i\ldots j}(y)$ and the antiperiodicity of the traction vector $\sigma_{ij}n_j$. It follows that:

$$\frac{1}{V}\int_V \sigma_{pq} a^{\alpha}_{pqi\ldots jk}(y)dV = \frac{1}{V}\int_V \sigma_{pk} X^{\alpha}_{pi\ldots j}(y)dV + \epsilon\frac{\partial}{\partial x_q}\left\{\frac{1}{V}\int_V \sigma_{pq} X^{\alpha+1}_{pi\ldots jk}(y)dV\right\} \tag{19}$$

Writing now this equation for $\alpha = 0,1,2,\ldots$ we obtain:

$$\begin{aligned}
\Sigma_{ij}(x) &= \frac{1}{V}\int_V \sigma_{ij}dV + \frac{\partial}{\partial x_q}\left\{\frac{\epsilon}{V}\int_V \sigma_{pq}X^1_{pij}(y)dV\right\}\\
T_{ijk}(x) &= \frac{h}{V}\int_V \sigma_{pk}X^1_{pij}(y)dV + \frac{\partial}{\partial x_q}\left\{\frac{h\epsilon}{V}\int_V \sigma_{pq}X^2_{pijk}(y)dV\right\}\\
M_{ijkl}(x) &= \frac{h^2}{V}\int_V \sigma_{pl}X^2_{pijk}(y)dV + \frac{\partial}{\partial x_q}\left\{\frac{h^2\epsilon}{V}\int_V \sigma_{pq}X^3_{pijkl}(y)dV\right\}
\end{aligned} \tag{20}$$

By combination of the above relations, we obtain:

$$\langle\sigma_{ij}\rangle_V = \Sigma_{ij}(x) - \frac{\partial T_{ijk}}{\partial x_k}(x) + \frac{\partial^2 M_{ijkl}}{\partial x_k \partial x_l}(x) - \cdots \tag{21}$$

The macroscopic balance equation reads then:

$$\frac{\partial \Sigma_{ij}}{\partial x_j}(x) - \frac{\partial^2 T_{ijk}}{\partial x_j \partial x_k}(x) + \frac{\partial^3 M_{ijkl}}{\partial x_j \partial x_k \partial x_l}(x) - \cdots + F_i(x) = 0 \tag{22}$$

which is exactly the balance equation of the general theory of gradient elastic media developed by Green and Rivlin (1964). When the series for the strain field is truncated at the first order, the macroscopic potential is given by (14) and the effective law only displays a relation between the macroscopic stress $\boldsymbol{\Sigma}(x)$ and the first hyperstress $\boldsymbol{T}(x)$ with the macroscopic strain, $\boldsymbol{E}(x)$ and the first gradient of strain, $\nabla\boldsymbol{E}(x)$. Higher order hyperstresses vanish and, in that case, the macroscopic balance equation reduces to:

$$\frac{\partial \Sigma_{ij}}{\partial x_j}(x) - \frac{\partial^2 T_{ijk}}{\partial x_j \partial x_k}(x) + F_i(x) = 0 \tag{23}$$

which is exactly the balance equation of first gradient elastic media.

It must be noted that Smyshlyaev and Cherednichenko (2000) developed a variational approach for deriving new higher-order effective relations for linear elastic composites which include the microstructural effects and the gradients of the macroscopic strain. By taking the variation of their elastic functional, Smyshlyaev and Cherednichenko (2000) observe that the balance equation does not reduce to the standard, Cauchy-type, one but introduces new additional terms. As mentioned by the authors themselves, the resulting balance equation may be recognized as the one introduced by the Toupin and Mindlin theories. However these additional terms introduce higher order homogenized stress tensors (which are only second-order tensors) but are not related to hyperstresses which are tensors of order 3, 4, etc. as in the present work.

4. Closed-form solutions for a stratified composite

As a first illustration we propose to derive the closed-form expressions for the components of gradient elasticity tensors in the case of a stratified composite. The material, depicted in Fig. 1, is constituted of two isotropic layers a and b, having the thickness $(1-\tau)h$ and τh with $0 \leqslant \tau \leqslant 1$. The volume fractions of phases a and b are respectively τ and $1-\tau$. The elastic moduli of the phase a are λ_1, μ_1 while those of the layer b are denoted λ_2 and μ_2. The layers a and b are periodically distributed along direction Oy_1. The material remains unchanged by any translation along directions Oy_2 and Oy_3 which implies that the local displacements at any given order are only functions of the variable y_1 (which is thereafter denoted y for simplicity). Still for simplicity reasons the "slow" variable x is omitted in the expression of the macroscopic quantities.

Exact expressions of functions $\boldsymbol{X}^1(y)$ and $\boldsymbol{X}^2(y)$, which are needed for the computation of effective elastic properties, have

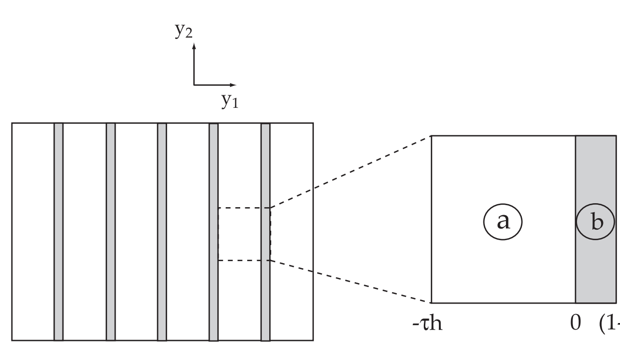

Fig. 1. The periodic unit cell for a stratified composite.

been already derived in Boutin (1996). However, due to the presence of misprints in the results, the corrected expressions are provided in Appendix B. We now provide the expressions for the higher order elasticity tensors. As for the case of fourth order tensors, a matricial representation is useful for representing tensorial operations on these tensors. The macroscopic strain, $\boldsymbol{E}$, can be represented by a vector of dimension 6, by using the modified Voigt notations:

$$\boldsymbol{E} = (E_1, \ldots, E_6) = \left(E_{11}, E_{22}, E_{33}, \sqrt{2}E_{23}, \sqrt{2}E_{13}, \sqrt{2}E_{12}\right) \tag{24}$$

Since the gradient of strain is symmetric according to its first two indices ($E_{ij,k} = E_{ji,k}$), it is possible to use a similar representation for $E_{ij,1}$, $E_{ij,2}$ and $E_{ij,3}$:

$$(E_{1,k}, \ldots, E_{6,k}) = \left(E_{11,k}, E_{22,k}, E_{33,k}, \sqrt{2}E_{23,k}, \sqrt{2}E_{13,k}, \sqrt{2}E_{12,k}\right) \tag{25}$$

with $k = 1,2,3$. Thus, the gradient of strain is represented by a vector of dimension 18:

$$\nabla\boldsymbol{E}(\boldsymbol{x}) = (E_{1,1}, \ldots, E_{6,1}, E_{1,2}, \ldots, E_{6,2}, E_{1,3}, \ldots, E_{6,3}) \tag{26}$$

The elasticity tensors $\boldsymbol{C}^{0,0}$, $\boldsymbol{C}^{0,1}$, $\boldsymbol{C}^{1,1}$, are represented by matrices of dimensions 6×6, 6×18 and 18×18:

$$\boldsymbol{C}^{0,0} = \begin{bmatrix} C_{11} & \ldots & C_{16} \\ & \ddots & \vdots \\ Sym & & C_{66} \end{bmatrix}_{6\times 6} \tag{27}$$

$$\boldsymbol{C}^{0,1} = \begin{bmatrix} C_{111} & \ldots & C_{161} & C_{112} & \ldots & C_{162} & C_{113} & \ldots & C_{163} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ C_{611} & \ldots & C_{661} & C_{612} & \ldots & C_{662} & C_{613} & \ldots & C_{663} \end{bmatrix}_{6\times 18} \tag{28}$$

$$\boldsymbol{C}^{1,1} = \begin{bmatrix} C_{1111} & \ldots & C_{1161} & C_{1112} & \ldots & C_{1162} & C_{1113} & \ldots & C_{1163} \\ & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ & & C_{6161} & C_{6112} & \ldots & C_{6162} & C_{6113} & \ldots & C_{6163} \\ & & & C_{1212} & \ldots & C_{1262} & C_{1213} & \ldots & C_{1263} \\ & & & & \ddots & \vdots & \vdots & \ddots & \vdots \\ & & & & & C_{6262} & C_{6213} & \ldots & C_{6263} \\ & & Sym & & & & C_{1313} & \ldots & C_{1363} \\ & & & & & & & \ddots & \vdots \\ & & & & & & & & C_{6363} \end{bmatrix}_{18\times 18} \tag{29}$$

Here we propose to restrict our analysis to these tensors; the identification of higher-order elasticity tensors requires the computation of functions $\boldsymbol{X}^i(y)$ for $i = 3,4,\ldots$ In the above matricial representation, coefficients C_{ij}, C_{ijk} and C_{ijkl} are computed from components $C^{0,0}_{ijpq}$, $C^{0,1}_{ijpqr}$ and $C^{1,1}_{ijkpqr}$ as follows:

$$C_{IP} = \alpha C^{0,0}_{ijpq}, \quad C_{IPr} = \alpha C^{0,1}_{ijpqr}, \quad C_{IkPr} = \alpha C^{1,1}_{ijkpqr} \tag{30}$$

where indices I, J and coefficient α are defined by:

$$I = \begin{cases} i & \text{if } i = j \\ 9 - i - j & \text{if } i \neq j \end{cases} \quad P = \begin{cases} p & \text{if } p = q \\ 9 - p - q & \text{if } p \neq q \end{cases}$$
$$\alpha = \begin{cases} 1 & \text{if } i = j \text{ and } p = q \\ \sqrt{2} & \text{if } i = j \text{ or } p = q \\ 2 & \text{if } i \neq j \text{ and } p \neq q \end{cases} \tag{31}$$

The coefficient α takes the values $\alpha = 1,\ \alpha = \sqrt{2}$ or $\alpha = 2$ depending on the values of the set $\{I,P\}$. The components of tensor $\boldsymbol{C}^{0,1}$ are null for symmetry reasons. The components of tensor $\boldsymbol{C}^{0,0}$ remain unchanged from the standard homogenization and are given in Boutin (1996). Components of tensor $\boldsymbol{C}^{1,1}$ are computed from (11) together with Eq. (5). The non null components of $\boldsymbol{C}^{1,1}$ are:

$$\begin{aligned}
C_{2222} &= C_{3333} = (1-\tau)^2\tau^2 \frac{Q_4^2 Q_2}{3Q_1^2} \\
C_{1212} &= C_{1313} = (1-\tau)^2\tau^2 \frac{(\lambda_2\mu_1 - \lambda_1\mu_2)^2 Q_2}{3(\lambda_2+2\mu_2)^2(\lambda_1+2\mu_1)^2 Q_1^2} \\
C_{2323} &= C_{3232} = (1-\tau)^2\tau^2 \frac{(\lambda_2 - \lambda_1)^2 \mu_1^2\mu_2^2 Q_2^3}{3(\lambda_2+2\mu_2)^2(\lambda_1+2\mu_1)^2 Q_1^2} \\
C_{5252} &= C_{6363} = (1-\tau)^2\tau^2 \frac{(\mu_1-\mu_2)^2 Q_3}{6\mu_1^2\mu_2^2 Q_2^2} \\
C_{6262} &= C_{5353} = (1-\tau)^2\tau^2 \frac{2(\mu_1-\mu_2)^2 Q_5}{3\mu_1^2\mu_2^2 Q_2^2} \\
C_{4242} &= C_{4343} = (1-\tau)^2\tau^2 \frac{(\mu_1-\mu_2)^2 Q_2}{6} \\
C_{1222} &= C_{1333} = (1-\tau)^2\tau^2 \frac{(\lambda_2\mu_1 - \lambda_1\mu_2) Q_4 Q_2}{3(\lambda_1+2\mu_1)(\lambda_2+2\mu_2) Q_1^2} \\
C_{1232} &= C_{1323} = (1-\tau)^2\tau^2 \frac{\mu_1\mu_2(\lambda_2-\lambda_1)(\lambda_2\mu_1 - \lambda_1\mu_2) Q_2^2}{3(\lambda_1+2\mu_1)^2(\lambda_2+2\mu_2)^2 Q_1^2} \\
C_{2232} &= C_{3323} = (1-\tau)^2\tau^2 \frac{\mu_1\mu_2(\lambda_2-\lambda_1) Q_4 Q_2^2}{3(\lambda_1+2\mu_1)(\lambda_2+2\mu_2) Q_1^2} \\
C_{2243} &= C_{3342} = (1-\tau)^2\tau^2 \frac{\sqrt{2}(\mu_2-\mu_1) Q_4 Q_2}{6Q_1} \\
C_{1243} &= C_{1342} = (1-\tau)^2\tau^2 \frac{\sqrt{2}(\lambda_2\mu_1 - \lambda_1\mu_2)(\mu_2-\mu_1) Q_2}{6(\lambda_1+2\mu_1)(\lambda_2+2\mu_2) Q_1} \\
C_{3243} &= C_{2342} = (1-\tau)^2\tau^2 \frac{\sqrt{2}\mu_1\mu_2(\mu_1-\mu_2)(\lambda_1-\lambda_2) Q_2^2}{6(\lambda_1+2\mu_1)(\lambda_2+2\mu_2) Q_1} \\
C_{5263} &= C_{6352} = (1-\tau)^2\tau^2 \frac{(\mu_1-\mu_2)^2 Q_3}{6\mu_1^2\mu_2^2 Q_2^2} \\
C_{5362} &= C_{6253} = (1-\tau)^2\tau^2 \frac{(\mu_1-\mu_2)^2 Q_6}{3\mu_1^2\mu_2^2 Q_2^2}
\end{aligned} \tag{32}$$

with:

$$\begin{aligned}
Q_1 &= \frac{1-\tau}{\lambda_1+2\mu_1} + \frac{\tau}{\lambda_2+2\mu_2} \\
Q_2 &= \frac{1-\tau}{\mu_1} + \frac{\tau}{\mu_2} \\
Q_3 &= (1-\tau)\mu_1 + \tau\mu_2 \\
Q_4 &= (\mu_2-\mu_1)Q_1 + (\lambda_2-\lambda_1)\frac{\mu_1\mu_2 Q_2}{(\lambda_1+2\mu_1)(\lambda_2+2\mu_2)} \\
Q_5 &= \frac{\mu_2(\mu_2+\lambda_2)}{\lambda_2+2\mu_2}\tau + \frac{\mu_1(\lambda_1+\mu_1)}{\lambda_1+2\mu_1}(1-\tau) \\
Q_6 &= \frac{\mu_2\lambda_2}{(\lambda_2+2\mu_2)}\tau + \frac{\mu_1\lambda_1}{\lambda_1+2\mu_1}(1-\tau)
\end{aligned} \tag{33}$$

Fig. 2 shows the variations of the components of the gradient elasticity tensor, given by (32), as functions of the volume fraction τ for materials whose elastic properties are given below. For brevity, only the "in plane" components have been plotted. It can be observed that all these higher order elastic coefficients become null when $\tau = 0$ and $\tau = 1$. In these two particular cases, the unit cell is constituted of a homogeneous medium, having the elastic properties λ_1, μ_1 or λ_2, μ_2. At the macroscopic scale, the strain gradient effects vanish and the constitutive relations are of Cauchy type with the elastic coefficients λ_1, μ_1 or λ_2, μ_2. For the applications proposed in Fig. 2 the following Poisson ratios have been used: $\nu_1 = 1/3$ and $\nu_2 = 1/4$. The Young's moduli are given by $E_1 = 10$ GPa and

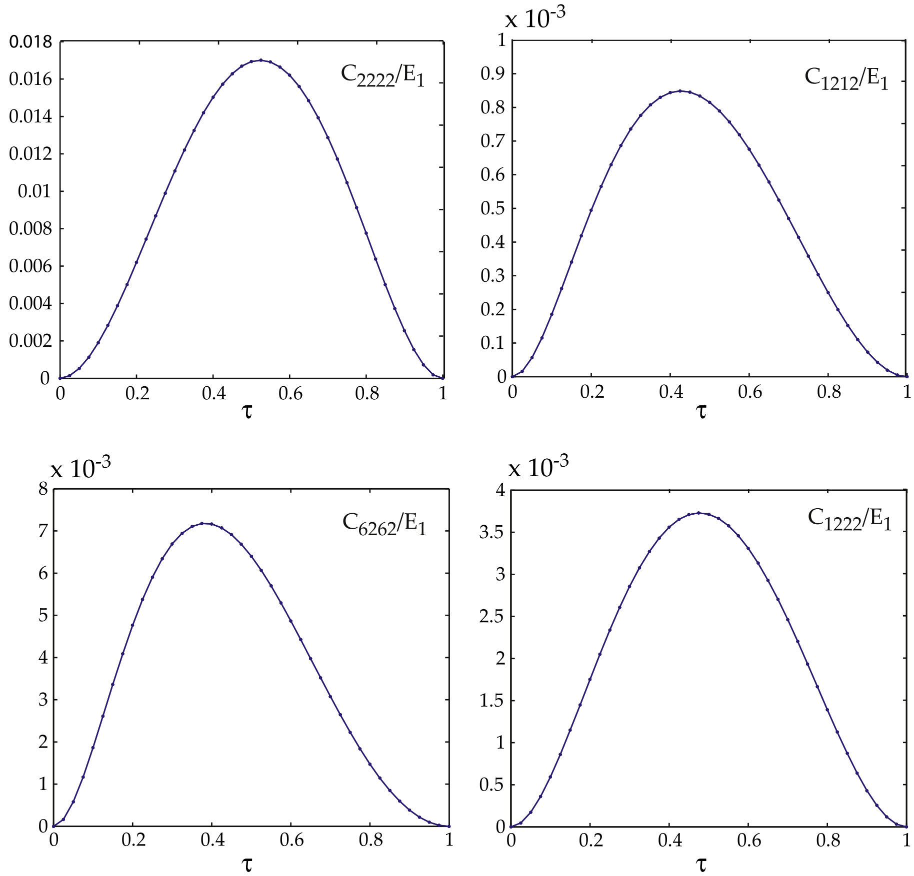

Fig. 2. Variations of the component C_{2222}, C_{1212}, C_{6262} and C_{1222} of the sixth-order elasticity tensor for the stratified medium with the volume fraction τ.

$E_2 = 20$ GPa. The gradient elastic coefficients represented in Fig. 2 have been normalized by the Young's modulus E_1. Note that in Bouyge et al. (2001), Kouznetsova et al. (2002) and Yuan et al. (2008), where higher order boundary conditions for the unit cell are used, the macroscopic behavior of the composite remains described by a gradient elasticity model even if at the local scale the material remains homogeneous. It is noteworthy that, at the contrary, the asymptotic expansion method combined with the energy based micro–macro transition described in the previous section leads to results for the gradient elastic properties which appear to be more physically realistic.

5. A FFT-based computational algorithm for computing the components of the sixth-order elasticity tensor

We aim now at deriving a FFT based numerical method for computing the effective elasticity tensors which enter the macroscopic law (12). As explained in Section 3.1, one has to compute functions $\boldsymbol{X}^1(y)$, $\boldsymbol{X}^2(y)$, $\boldsymbol{X}^3(y), \ldots$ by solving the hierarchy of elasticity problems provided in Appendix A. To this end, and along the lines of the paper of Moulinec and Suquet (1994), we first propose to derive the Lippmann–Schwinger integral equation associated to the higher-order homogenization problems, which is the basis of the FFT-based iterative scheme. Indeed, the integral equation described in Moulinec and Suquet (1994) is only applicable for the 0-order homogenization problem (corresponding to $\boldsymbol{g}^0(y) = 0$ and $\boldsymbol{p}^0(y) = \boldsymbol{c}(y) : \boldsymbol{E}$) and must be generalized for handling problems dealing with arbitrary expressions for the body force $\boldsymbol{g}(y)$ and the polarization $\boldsymbol{p}(y)$ (here and in the next of the paper the variable x is omitted for simplicity).

5.1. The Lippmann–Schwinger equation associated to higher-order homogenization problems

Let us introduce in (A.1) a homogeneous reference medium with the elasticity tensor $\boldsymbol{c}^0$. The stress–strain relation can be rewritten as:

$$\boldsymbol{\sigma}(y) = \boldsymbol{c}^0 : \boldsymbol{\varepsilon}(y) + \boldsymbol{\tau}(y) \tag{34}$$

where $\boldsymbol{\tau}(y)$ is defined as:

$$\boldsymbol{\tau}(y) = (\boldsymbol{c}(y) - \boldsymbol{c}^0) : \boldsymbol{\varepsilon}(y) + \boldsymbol{p}(y) \tag{35}$$

Taking now the Fourier transform, defined, for any Y-periodic function $F(y)$, by:

$$F(\xi) = \mathcal{F}(F(y)) = \frac{1}{V}\int_V F(x)\exp(i\xi \cdot \boldsymbol{x})dx \tag{36}$$

the elasticity problem reads:

$$\begin{cases} i\boldsymbol{\sigma}(\xi).\xi + \boldsymbol{g}(\xi) = 0 \\ \boldsymbol{\sigma}(\xi) = \boldsymbol{c}^0 : \boldsymbol{\varepsilon}(\xi) + \boldsymbol{\tau}(\xi) \\ \boldsymbol{\varepsilon}(\xi) = \frac{i}{2}(\boldsymbol{\xi} \otimes \boldsymbol{u}(\xi) + \boldsymbol{u}(\xi) \otimes \boldsymbol{\xi}) \end{cases} \tag{37}$$

Let us now introduce $\theta(\xi)$ defined by:

$$\boldsymbol{\theta}(\xi) = \frac{i}{\|\xi\|^4}\left[\boldsymbol{\xi} \otimes \boldsymbol{\xi}\boldsymbol{g}(\xi).\boldsymbol{\xi} - (\boldsymbol{g}(\xi) \otimes \boldsymbol{\xi} + \boldsymbol{\xi} \otimes \boldsymbol{g}(\xi))\|\boldsymbol{\xi}\|^2\right] \tag{38}$$

and such that $\boldsymbol{g}(\xi) \cdot \xi = i\theta(\xi)$. The solution is:

$$\boldsymbol{\varepsilon}(\xi) = -\boldsymbol{\Gamma}^0(\xi) : (\boldsymbol{\tau}(\xi) + \boldsymbol{\theta}(\xi)) \tag{39}$$

or equivalently, in the real space:

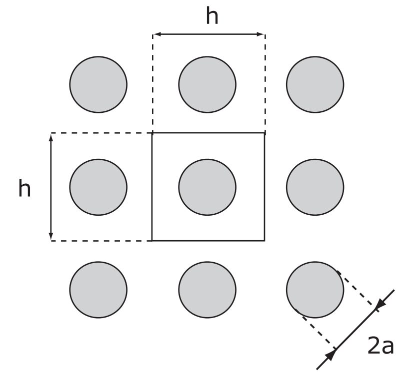

Fig. 3. Regular array of cylindrical inclusions aligned along direction Ox_3.

$$\boldsymbol{\varepsilon}(y) = -\boldsymbol{\Gamma}^0(y) * (\boldsymbol{\tau}(y) + \boldsymbol{\theta}(y)) \tag{40}$$

where $\boldsymbol{\Gamma}^0$ represent the Green operator for the strain and the symbol "$*$" denotes the convolution product. Finally, replacing $\boldsymbol{\tau}(\xi)$ by its expression given by (35), the solution of (A.1) complies with the following integral equation:

$$\boldsymbol{\varepsilon}(y) = -\boldsymbol{\Gamma}^0(y) * \left[(\boldsymbol{c}(y) - \boldsymbol{c}^0) : \boldsymbol{\varepsilon}(y) + \boldsymbol{p}(y) + \boldsymbol{\theta}(y)\right] \tag{41}$$

5.2. The FFT based algorithm

Similarly to Moulinec and Suquet (1994), we propose to search the solution of Lippmann–Schwinger Eq. (41) by means of the following iterative scheme:

$$\boldsymbol{\varepsilon}^{i+1}(\xi) = -\boldsymbol{\Gamma}^0(\xi) * \left[(\boldsymbol{c}(y) - \boldsymbol{c}^0) : \boldsymbol{\varepsilon}^i(y) + \boldsymbol{p}(y) + \boldsymbol{\theta}(y)\right] \tag{42}$$

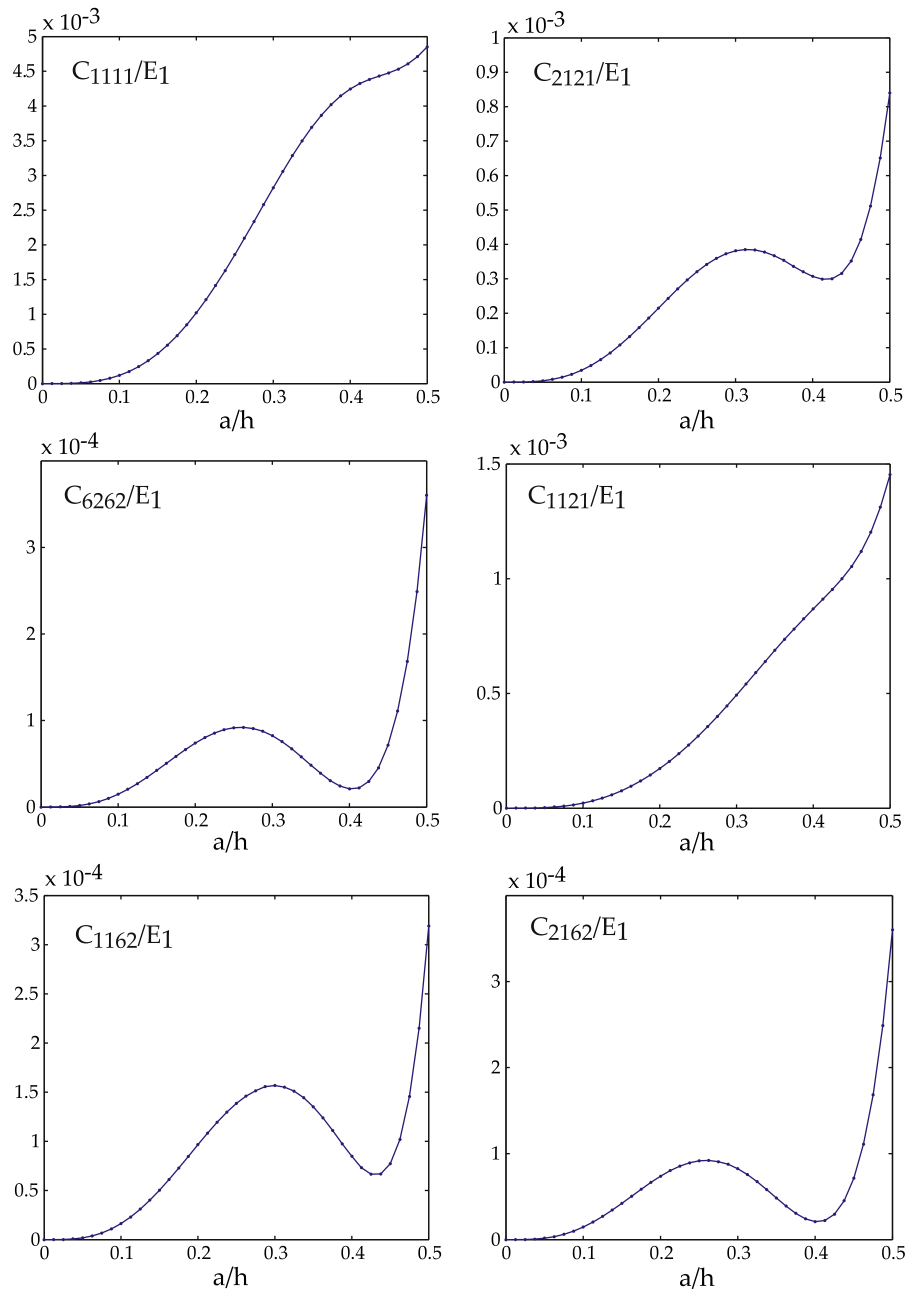

Fig. 4. Variations of the component C_{1121}, C_{2121}, C_{1121}, C_{6262}, C_{1162}, C_{2162} of the sixth-order gradient elasticity tensor as a function of a/h for the fiber-reinforced composite.

the scheme starting from $\boldsymbol{\varepsilon}^1 = 0$. A simplification of the above recurrence relation is possible. Since the tensors $\boldsymbol{\varepsilon}^i(y)$ is compatible and $\langle \boldsymbol{\varepsilon}^i(y)\rangle_V = 0$ at each iteration i, it follows that:

$$\boldsymbol{\Gamma}^0(\xi) * \left[\boldsymbol{c}^0 : \boldsymbol{\varepsilon}^i(y)\right] = \boldsymbol{\varepsilon}^i(y) \tag{43}$$

Consequently:

$$\boldsymbol{\varepsilon}^{i+1}(y) = \boldsymbol{\varepsilon}^i(y) - \boldsymbol{\Gamma}^0(\xi) * \left[\boldsymbol{c}(y) : \boldsymbol{\varepsilon}^i(y) + \boldsymbol{p}(y) + \boldsymbol{\theta}(y)\right] \tag{44}$$

The following iterative scheme is then employed:

$$\begin{aligned} &\boldsymbol{\varepsilon}^i(y) = \mathcal{F}^{-1}(\boldsymbol{\varepsilon}^i(\xi)) \\ &\boldsymbol{\varepsilon}^i(y) = \boldsymbol{c}(y) : \boldsymbol{\varepsilon}^i(y) + \boldsymbol{p}(y) \\ &\boldsymbol{\sigma}^i(\xi) = \mathcal{F}(\boldsymbol{\sigma}^i(y)) \end{aligned} \tag{45}$$

convergence test

$$\boldsymbol{\varepsilon}^{i+1}(\xi) = \boldsymbol{\varepsilon}^i(\xi) - \boldsymbol{\Gamma}^0(\xi) : (\boldsymbol{\sigma}^i(\xi) + \boldsymbol{\theta}(\xi)).$$

The exact Fourier transform is thereafter approximated by the finite discrete Fourier transform which is computed by using the FFT algorithm. The iterative scheme is stopped when the stress field complies with the local equilibrium. The following convergence test has been used in our computations:

$$\frac{\|\boldsymbol{P}(\xi) : \boldsymbol{\sigma}^i(\xi) + \boldsymbol{\theta}(\xi)\|}{\|\boldsymbol{\sigma}^i(\xi)\|} < h. \tag{46}$$

where $\|\bullet\|$ denotes the Frobenius norm and $\boldsymbol{P}(\xi)$ is the fourth order tensor defined by $\boldsymbol{P}(\xi) = \boldsymbol{I} - \boldsymbol{Q}(\xi)$ and $Q_{ijpq}(\xi) = (k_{ip}k_{jq} + k_{iq}k_{jp})/2$ and $k_{ij} = \delta_{ij} - \xi_i\xi_j/\|\xi\|^2$. Tensors $\boldsymbol{P}(\xi)$ and $\boldsymbol{Q}(\xi)$ are two projectors; for any second-order tensor $\boldsymbol{a}$, $\boldsymbol{Q}(\xi) : \boldsymbol{a}$ is interpreted as the projection of $\boldsymbol{a}$ along the plane orthogonal to the wave-vector ξ whereas $\boldsymbol{P}(\xi) : \boldsymbol{a}$ is the out of plane projection of $\boldsymbol{a}$. Following Moulinec and Suquet (1994), the reference medium, giving the convergence of the FFT-based iterative scheme, is chosen as:

$$\boldsymbol{c}^0 = \frac{1}{2}\left[\max_y \boldsymbol{c}(y) + \min_y \boldsymbol{c}(y)\right] \tag{47}$$

5.3. Illustration of the method

As an illustration purpose we compute the higher-order elastic coefficients in the case of a composite made up of long fibers with a circular cross section. The sections of the fibers are assumed to be arranged along a periodic squared lattice (see Fig. 3). For the calculations, a squared unit cell has been considered and a representation with a grid containing 128×128 points has been used for effecting the Fourier transform and its inverse. The width of the cell is denoted by h and the radius of the cylinder is denoted by a. The elastic moduli of the matrix are λ_1, μ_1 whereas those of the fibers are denoted by λ_2, μ_2. For all applications, the values of the elastic moduli are the ones already used in the previous section.

Plane strain conditions are considered; it follows that only the components $E_{ij,k}$ with $i, j, k = 1, 2$ are used. Due to the symmetry of the unit cell, the relation giving the components of the hyperstress $\boldsymbol{T}$ as functions of the components of the macroscopic gradient of strain $\nabla\boldsymbol{E}$ is:

$$\begin{pmatrix} T_{11} \\ T_{21} \\ T_{62} \\ T_{22} \\ T_{12} \\ T_{61} \end{pmatrix} = h^2 \begin{pmatrix} C_{1111} & C_{1121} & C_{1162} & 0 & 0 & 0 \\ C_{1121} & C_{2121} & C_{2162} & 0 & 0 & 0 \\ C_{1162} & C_{2162} & C_{6262} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{1111} & C_{1121} & C_{1162} \\ 0 & 0 & 0 & C_{1121} & C_{2121} & C_{2162} \\ 0 & 0 & 0 & C_{1162} & C_{2162} & C_{6262} \end{pmatrix} \begin{pmatrix} E_{1,1} \\ E_{2,1} \\ E_{6,2} \\ E_{2,2} \\ E_{1,2} \\ E_{6,1} \end{pmatrix} \tag{48}$$

where the compact notation for the components of the hyperstress and strain-gradient are used. The fourth-order elasticity tensor can be obtained from usual homogenization procedures and its coefficients are not reported here. Relation (48) involves only six elastic coefficients. The variation of these coefficients with ratio a/h are shown in Fig. 4. It can be observed that the gradient elastic coefficients are again null when $a = 0$, corresponding to the case of a unit cell having the constant elastic moduli λ_1 and μ_1, whereas these coefficients are maximal when the ratio a/h is maximal and equal to 1/2, the composite being still heterogeneous in this last case. The changes with concentration of theses coefficients are monotonous for C_{1111} and C_{1121} while they are characterized by a minimum between a/h equal to 0.3 and 0.5 for all other coefficients.

6. Conclusion

In this paper we have proposed a simple and efficient method for the determination of the gradient elastic properties of periodic composite materials. The approach can be summarized as follows: (i) the elastic solution is expanded along a series expansion for which higher order terms are kept (in addition to those generally considered in the usual homogenization framework) (ii) the elastic energy of the equivalent homogeneous material is computed by means of a generalized Hill–Mandel lemma, (iii) the constitutive relations are derived from the "state law" associated with this macroscopic potential.

The averaging rule giving the higher-order elasticity tensors have been derived. The components of these higher-order elasticity tensors are obtained by solving higher-order homogenization problems for the unit cell of the periodic medium. Closed-form solutions for these higher-order elasticity tensors are provided in the particular case of a stratified composite. For arbitrary microstructures, a computational method has been developed in the last part of the paper. The method of resolution uses an iterative scheme and the exact expression of the Green's operator in the Fourier space. The relevance of this approach has been illustrated in the case of a periodic array of elastic fibers embedded in an elastic matrix.

This work opens the way to many new applications and extensions not only in the domain of linear but also in the domain of non linear homogenization. For instance, the determination of gradient properties of elastic or plastic polycrystalline materials is an array of research of high importance. The extension of our approach in this context will be the scope of a future work.

Appendix A. Hierarchy of problems

The hierarchy of linear elastic problems, leading to the identification of tensors $\boldsymbol{X}^\alpha(y)$ for $\alpha = 1, 2, 3, \ldots$, can be put into the form:

$$\begin{cases} \nabla_y \cdot \boldsymbol{\sigma}(y) + \boldsymbol{g}^\alpha(y) = 0 \\ \boldsymbol{\sigma}(y) = \boldsymbol{c}(y) : \boldsymbol{\varepsilon}(y) + \boldsymbol{p}^\alpha(y) \\ \boldsymbol{\varepsilon}(y) = \frac{1}{2}(\nabla_y \otimes \boldsymbol{u}(y) + \boldsymbol{u}(y) \otimes \nabla_y) \\ \boldsymbol{u}(y)\text{periodic},\ \langle \boldsymbol{u}(y)\rangle_V = 0,\ \boldsymbol{t} = \boldsymbol{\sigma}(y) \cdot \boldsymbol{n}\ \text{antiperiodic} \end{cases} \tag{A.1}$$

In which the coordinate x is omitted for simplicity. Expressions of $\boldsymbol{g}^\alpha(y)$ and $\boldsymbol{p}^\alpha(y)$ are:

$$\begin{aligned} &\text{order } 0: \begin{cases} \boldsymbol{g}^0(y) = 0 \\ \boldsymbol{p}^0(y) = \boldsymbol{c}(y) : \boldsymbol{E} \end{cases} \\ &\text{order } 1: \begin{cases} \boldsymbol{g}^1(y) = \left[\boldsymbol{c}^0(y) - \beta(y)\langle \boldsymbol{c}^0(y)\rangle_V\right] : \cdot\nabla\boldsymbol{E} \\ \boldsymbol{p}^1(y) = \frac{1}{2}\boldsymbol{c}(y) : \left[\boldsymbol{X}^1(y) : \nabla\boldsymbol{E} + (\boldsymbol{X}^1(y) : \nabla\boldsymbol{E})^t\right] \end{cases} \\ &\text{order } 2: \begin{cases} \boldsymbol{g}^2(y) = \left[\boldsymbol{c}^1(y) - \beta(y)\langle \boldsymbol{c}^1(y)\rangle_V\right] :: \nabla^2\boldsymbol{E} \\ \boldsymbol{p}^2(y) = \frac{1}{2}\boldsymbol{c}(y) : \left[\boldsymbol{X}^2(y) : \cdot\nabla^2\boldsymbol{E} + (\boldsymbol{X}^2(y) : \cdot\nabla^2\boldsymbol{E})^t\right] \end{cases} \\ &\text{etc.} \end{aligned} \tag{A.2}$$

where $\beta(y)$ is given by:

$$\beta(y) = \frac{\rho(y)}{\langle \rho(y) \rangle_V} \tag{A.3}$$

When the body force is of the type: $\boldsymbol{f}(x,y) = \rho(y)\boldsymbol{f}^0(x)$, $\rho(y)$ being the density of the material constituents. The solutions of these linear elastic problems for $\alpha = 0, 1, 2$, etc. are:

$$\begin{aligned} &\text{order } 0: \ \boldsymbol{u} = \boldsymbol{X}^1(y) : \boldsymbol{E} \\ &\text{order } 1: \ \boldsymbol{u} = \boldsymbol{X}^2(y) : \cdot\nabla\boldsymbol{E} \\ &\text{order } 2: \ \boldsymbol{u} = \boldsymbol{X}^3(y) :: \nabla^2\boldsymbol{E} \\ &\text{etc.} \end{aligned} \tag{A.4}$$

where tensors $\boldsymbol{X}^1(y)$, $\boldsymbol{X}^2(y)\boldsymbol{X}^3(y)$ are localization tensors which do not depend on macroscopic variables $\boldsymbol{E}, \nabla\boldsymbol{E}$ and $\nabla^2\boldsymbol{E}$, but depend only on the microstructure, as in the classical homogenization framework.

Appendix B. Solution for a stratified composite

For simplicity, the variable y_1 is denoted thereafter by y. The solution at the first order involves the components of the third order tensor $\boldsymbol{X}^{(1)}(y)$ which are:

$$\begin{aligned} X^1_{111}(y) &= kf(y) \\ X^1_{122}(y) &= X^1_{133}(y) = k[D(\lambda)/D(\lambda+2\mu)]f(y) \\ X^1_{212}(y) &= X^1_{313}(y) = mf(y) \end{aligned} \tag{B.1}$$

where function $f(y)$ is given by:

$$f(y) = \begin{cases} [y/h - (1-\tau)/2]/(1-\tau) & \text{in layer } a \\ -[y/h + \tau/2]/\tau & \text{in layer } b \end{cases} \tag{B.2}$$

coefficients k and m are given by:

$$\begin{aligned} k &= H(\lambda+2\mu)D(1/(\lambda+2\mu)) \\ m &= H(\mu)D(1/\mu) \end{aligned} \tag{B.3}$$

in which $H(\psi)$ and $D(\psi)$ are given, for any ψ, by:

$$\begin{aligned} H(\psi) &= \left[\tfrac{1-\tau}{\psi_a} + \tfrac{\tau}{\psi_b}\right]^{-1} \\ D(\psi) &= \tau(1-\tau)(\psi_a - \psi_b) \end{aligned} \tag{B.4}$$

where ψ_a and ψ_b are respectively the values of ψ in layer a and in layer b. The solution at the second order involves the components of $\boldsymbol{X}^2(\boldsymbol{y})$ which are:

$$\begin{aligned} X^2_{1111}(y) &= hk(\langle F\rangle - F)X^2_{1221}(y) = X^2_{1331}(y) \\ &= hk(\langle F\rangle - F)D(\lambda)/D(\lambda+2\mu)X^2_{1122}(y) = X^2_{1133}(y) \\ &= hm(\langle \eta F\rangle - \eta F)X^2_{2112}(y) = X^2_{3113}(y) \\ &= hk(\langle F\rangle - F) + (\langle F/\mu\rangle - F/\mu)H(\lambda \\ &\quad + 2\mu)D(\eta)X^2_{2222}(y) \\ &= X^2_{3333}(y) \\ &= hk(\langle F\rangle - F)D(\lambda)/D(\lambda+2\mu) + (\langle F/\mu\rangle - F/\mu)H(\lambda \\ &\quad + 2\mu)D(\phi)X^2_{2332}(y) \\ &= X^2_{3223}(y) \\ &= hk(\langle F\rangle - F)D(\lambda)/D(\lambda+2\mu) + (\langle F/\mu\rangle - F/\mu)H(\lambda \\ &\quad + 2\mu)D(\gamma)X^2_{2121}(y) \\ &= X^2_{3131}(y) = hm(\langle F\rangle - F)X^2_{2233}(y) = X^2_{3322}(y) \\ &= h(\langle F/\mu\rangle - F/\mu)D(\mu) \end{aligned} \tag{B.5}$$

where function $F(y)$ is defined by:

$$F(y) = \begin{cases} y[y/h - (1-\tau)]/2(1-\tau) & \text{in layer } a \\ -y[y/h + \tau]/2\tau & \text{in layer } b \end{cases} \tag{B.6}$$

and the following notations have been used:

$$\begin{aligned} M(\psi) &= (1-\tau)\psi_a + \tau\psi_b \\ \eta &= \lambda/(\lambda+2\mu) \\ \gamma &= M(\eta)\eta + \lambda(1-\eta)/H(\lambda+2\mu) \\ \phi &= \gamma + 2\mu/H(\lambda+2\mu) \end{aligned} \tag{B.7}$$

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